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New challenges in integrated water quality modelling

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Abstract:

There is an increasing pressure for development of integrated water quality models that effectively couple catchment and in-stream biogeochemical processes. This need stems from increasing legislative requirements and emerging demands related to contemporary climate and land use changes. Modelling water quality and nutrient transport is challenging due a number of serious constraints associated with the input data as well as existing knowledge gaps related to the mathematical description of landscape and in-stream biogeochemical processes. The present paper summarizes the discussions held during the workshop on 'Integrated water quality modelling: future demands and perspectives' (Magdeburg, Germany, 23–24 June 2008). Our primary focus is placed on the current limitations and future challenges in water quality modelling. In particular, we evaluate the current state of integrated water quality modelling, we highlight major research needs to assess and reduce model uncertainties, and we examine opportunities to enhance model predictive capacity. To better account for the need of upscaling process knowledge, we advocate the adoption of combined process-oriented field and modelling studies at representative sites. In-stream nutrient metabolism investigations at the entire range of stream and river scales will enable the improvement of the mathematical representation of these processes and therefore the articulation level of coupled watershed-receiving waterbody models. Keeping the complexity of integrated water quality models in mind, the development of novel uncertainty analysis techniques for rigorous assessing parameter identification and model credibility is essential. In this regard, we recommend the use of Bayesian calibration frameworks that explicitly accommodate measurement errors, parameter uncertainties, and model structure errors. The Bayesian inference can be used to quantify the information the data contain about model inputs, to offer insights into the covariance structure among parameter estimates, to obtain predictions along with credible intervals for model outputs, and to effectively address the 'change of support' problems. Copyright © 2010 John Wiley & Sons, Ltd.

KEY WORDS integrated water quality modelling; nutrient fate and transport; hyporheic zone processes; uncertainty analysis; equifinality; Bayesian inference techniques

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INTRODUCTION

Environmental policy making and successful management implementation require robust methods for assessing the contribution of various point and non-point pollution sources to water quality problems as well as methods for estimating the expected and achieved compliance with the water quality goals. Water quality models have been widely used for creating the scientific basis for environmental management decisions by providing a predictive link between management actions and ecosystem response (Arhonditsis *et al*., 2006). Integrated catchment management is becoming an increasingly common legislative requirement under the Water Framework Directive (WFD) in the European Union or the Clean Water Act in the United States. Analyses of water quality management scenarios invite the development of predictive models, which should be process-based and (ideally) integrated with hydrological models that quantitatively describe the spatiotemporal patterns of the transporting medium (e.g. water flow rates). Ultimately, linking land use practises to the in-stream nutrient concentrations and then accounting for the interplay among physical, chemical, and biological processes is necessary to control cultural eutrophication (Conley *et al*., 2009).

Water quality models aim to describe the spatiotemporal dynamics of constituents of concern. A number of components or state variables have been gradually incorporated into models over the past seven decades following the evolution of water quality problems. Generally, water quality models are classified according to their complexity, application domain (catchment, receiving water body, or integrated models), and type of water quality variables predicted (e.g. nutrients, sediments, dissolved oxygen) (Borah *et al*., 2006). The data requirements for water quality models increase with the complexity and scope of application and can be specific to the management question at hand. Despite the significance and considerable attention, experiences from different national projects worldwide revealed that the

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available water quality models are not always reliable tools for operational applications by water resource managers. For example, applications of different models in the same river can support predictions of nutrient concentrations that may differ by more than 100% and sometimes project system responses that are contradictory (Bouraoui *et al*., 2009; Hejzlar *et al*., 2009; Kronvang *et al*., 2009; Schoumans *et al*., 2009). Thus, an imperative challenge in integrated water quality modelling is to delve into the crux of the unresolved weaknesses and to pinpoint some of the future thrusts in progress.

One of the critical problems in catchment-scale water quality modelling is to accommodate the substantial spatial variability that frequently dominates the catchment behaviour. The so-called distributed water quality models aim to adequately represent this heterogeneity through a sensibly refined spatial resolution (Refsgaard, 2007). Catchment modelling is further complicated by the need to describe the water and mass fluxes and transformation processes in different compartments like the soil, vadose and saturated zones as well as the surface water transportation processes including stream-aquifer interactions. The upscaling from field-scale to larger scale patterns by simply describing processes in a spatially distributed way is commonly termed bottom-up, mechanistic, or reductionistic (Ebel and Loague, 2006). Although such a reductionistic approach is made possible through advancements in computer technology, its scientific foundation is at least controversial. Important reasons for that are the non-linear interactions between transport and transformation, the increasing problems of parameter identifiability, and the lack of a spatially distributed evaluation of the (sub)models (Beven, 1993; Wagener, 2003; Woods, 2003; Wagener and Gupta, 2005). The upscaling problems are also due to the fact that a well-accepted upscaling methodology for transferring microscale processes to the mesoscale is still missing (Wagener *et al*., 2007). This is not only true for catchment processes but also for in-stream processes. For example, it has been recently demonstrated that serious artefacts can result from inappropriate scale-transition methodologies in coupled hydrological–biogeochemical modelling of pollutants spreading through the groundwater–surface water interface (Lindgren and Destouni, 2004; Darracq and Destouni, 2005; Destouni and Darracq, 2006).

The accurate quantification of the overland nutrient transport (Isermann, 1990; Kronvang *et al*., 1995) and the subsequent in-stream attenuation processes are essential for predicting nutrient delivery rates to downstream inland and coastal waters (Darracq and Destouni, 2007). In particular, several studies argue that the magnitude of the in-stream mass transformation processes may be a key factor for the delineation of sensitive areas within watersheds (Alexander *et al*., 2000; Seitzinger *et al*., 2002; Withers and Jarvie, 2008). It is also suggested that the hyporheic zone has an important impact on these transformation processes, although the quantitative assessment for a given river is still difficult and highly uncertain (Jones and Mulholland, 2000; Birgand *et al*., 2007). Closely related to the improvement of the quantitative description of catchment and in-stream processes along with the aforementioned scale-transition methodologies are open questions on model integration between catchment and in-stream submodels. Many process-based studies have focussed on exchange between surface water bodies (lakes, streams) and groundwater (Hayashi and Rosenberry, 2002; Sebestyen and Schneider, 2004; Harvey *et al*., 2005), but only few attempts have been made to closely link terrestrial water fluxes with the surface waters of the entire river network of larger catchments (Migliaccio *et al*., 2007; Rassam *et al*., 2008). It is also unclear what the appropriate model linkage strategies are and how can we ensure transparency of complex integrated models.

The continuous demand to include as much knowledge as possible in 'state-of-the-art' hydrological and in-stream water quality models inevitably results in considerably more complex model structures (Beck, 1999; Omlin and Reichert, 1999). Although the increase of the articulation level of our models is certainly the way forward, it should also be acknowledged that the increasing complexity reduces our ability to properly constrain the parameters from observations, for example, the number of parameters in planktonic models that must be specified from the data is approximately proportional to the square of the number of compartments (Denman, 2003). Furthermore, while a more detailed process description supposedly decreases the structural uncertainties of the models (Snowling and Kramer, 2001; Lindenschmidt, 2006), the actual impact of the growing complexity should be evaluated by examining alternative process descriptions or, less ideally, by adding correlated noise to model structures (Van Griensven and Meixner, 2004). Compared with hydrological models, the problem of uncertainty is further accentuated with the biogeochemical catchment and/or in-stream water quality models. Because process-based river water quality models in general describe biological mechanisms like phytoplankton growth or grazing by zooplankton, they are typically characterized by higher complexity and larger number of parameters, and therefore the equifinality problem is accentuated (Arhonditsis *et al*., 2006; Beven, 2006). Thus, a critical decision when selecting and/or developing a water quality model is the determination of the optimal model complexity for evaluating the effects of the potential management actions with an acceptable level of uncertainty.

This paper is a synthesis of discussions held during the workshop on 'Integrated water quality modelling: future demands and perspectives' in connection with the EU funded Marie Curie ToK Project 'Modelling Competence' (Magdeburg, Germany, 23–24 June 2008). In particular, this workshop aimed (i) to evaluate the current state of integrated water quality modelling, (ii) to pinpoint major research needs that should enhance the predictive capacity of the present generation of water quality models, (iii) to rigorously assess model uncertainties, and (iv) to highlight the future directions for

Figure 1. Surface runoff and inundation in a flat area (Beltrum, Netherlands) with coarse sandy soils (Courtesy: Willemijn Appels (left) and Ype van der Velde (right), Wageningen University)

improving model-based environmental management. The paper is structured into four major topics as follows:

- catchment water quality modelling involving both small- and regional-scale, process-oriented biogeochemical modelling;
- in-stream water quality modelling with special emphasis on hyporheic zone processes and biogeochemical controls;
- linkages between catchment and receiving water body models; and
- uncertainties in water quality modelling.

CATCHMENT WATER QUALITY MODELLING

Enormous advances have been made in catchment-scale modelling over the past decades. The scientific and operational success of such modelling endeavours, however, may obscure fundamental shortcomings that we have to be aware of. In this paper, we will elaborate on few particularly problematic aspects of the catchment water quality modelling, as they have emerged from our past experience and contemporary practice.

Are we considering the correct scales in distributed modelling?

In all earth sciences, the perception of scale is an intrinsic aspect of both experimental and modelling research. Adhering to McLaughlin and van Geer's (1992, personal communication) scale typology, we distinguish among the scales of the (i) involved process(es); (ii) observations and measurements; (iii) model discretization; and (iv) governance and management. In distributed models, the typical model resolution level and data availability are pragmatically determined by cost limitations and computational demands, which implies that model discretization usually differs from the existing measurements and can be coarse relative to the actual scales of the driving processes. A characteristic example involves the scale of processes that typically control surface water quality which may be determined by localized phenomena, such as the surface runoff. The latter process can be envisioned as a superficial ephemeral stream flow, where most water is concentrated in small streams that occupy only a minor part of the soil surface and therefore accounts for only a minor fraction of the discretization surface/volume size. (Both redistributed water and localized flow into a ditch can be seen in Figure 1.) To deal with such scale mismatch problems, it seems inevitable that new modelling concepts should be developed to effectively link the different scales.

How accurate is the representation of specific hydrological processes (preferential flow, surface runoff)?

Regarding the difference between process and modelling scales, the typical coarseness of discretization of numerical models implies that the preferential flow is depicted in a lumped form in the model equations. Many fundamental insights and experimental illustrations have been offered into the preferential flow and transport, while the analytical expressions derived can provide guidelines for discretization, large-scale process formulations, and equivalent parameterization of the upscaled model parameters (Rinaldo and Marani, 1987; Dagan, 1989; Cirpka *et al*., 1999; Hesse *et al*., 2009). Hence, the scientific toolkit is not empty to appropriately model at different discretization scales, although there is little doubt that more empirical studies are needed in offering practical consultation when delineating the optimal aggregation level. In some cases, the local-scale processes are still hardly understood, inadequately translated in model equations, and poorly parameterized. Preferential flow and transport, especially when it involves dual permeability domains, is an example where each study site requires a completely new parameterization. Needless to say, that the existing information for such site-specific parameterizations is rarely sufficient. New examples of channelled flow, for example, the pin and sand boils, discovered by De Louw (2007) have received little consideration in modelling. In particular, it has been shown that these boils can transport substantial amount of water (often rich of salts and nutrients) or both water and (fluidized) sand from deeper layers to surface water where little craters may form. Yet, these processes have neither been integrated in surface water quality modelling

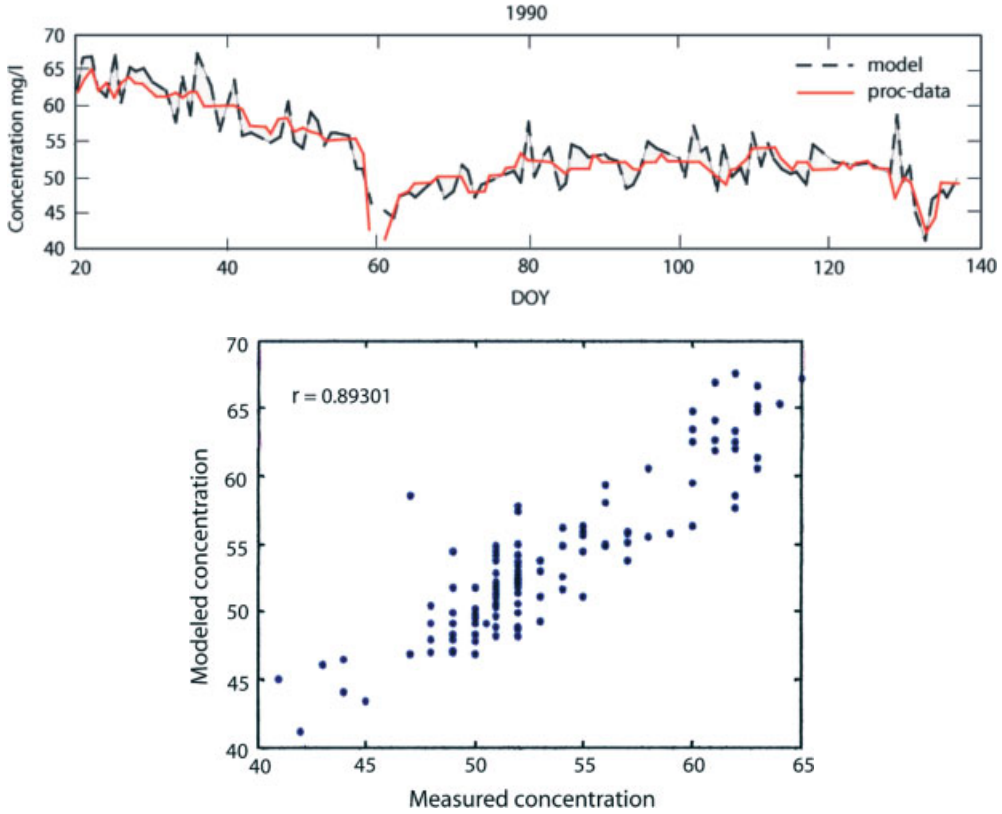

Figure 2. Measured and predicted chloride concentrations as a function of the day of year (DOY) for the Hupsel Brook experimental catchment in the east of the Netherlands. Predicted values were obtained by inverse modelling of the original MRF approach by Van der Ploeg and van Wijnen (2009)

nor have they been parameterized properly, except by inverse modelling exercises (De Louw, 2007).

Are we giving enough consideration to temporal variability?

Because of their simple structure and good description obtained, the hydrographs relating rainfall inputs to stream discharges are a popular concept in hydrology. The premise of such impulse–response relationships is founded upon the assumption of linear and time-invariant properties of the underlying catchment. However, the time-invariance assumption is questionable and a characteristic example of its limited applicability is the mass response function (MRF) developed by Rinaldo and Marani (1987) and Rinaldo *et al.* (1989) to characterize the flow and (solute, mass) transfer for entire watersheds or river basins. We implemented their approach for the Hupsel catchment in the Netherlands, which is a small, 650 ha size catchment in the east of the country (for a good description, see Van der Velde *et al.*, 2009a). Unfortunately, our inverse modelling of the MRF gave only moderately satisfactory results (Van der Ploeg and van Wijnen, 2009). The underlying reason is that temporal variability of stream discharge is significant, as prolonged dry (summer) periods tend to result in low stream flows, or even dry ditches and brooks, whereas wet periods are associated with nearly filled streams and close to inundation conditions (Arhonditsis *et al.*, 2002, Van der Velde *et al.*, 2009b). If, however, we are able to obtain different MRFs for the two main periods of the year (dry summer and wet winter half years, respectively), the time-dependent parameterization can provide acceptable results (Figure 2). Similar assumptions can be made with regards to the seasonal trends in other climate zones and geohydrological conditions, while the wealthy literature on 'old' and 'new' water (usually non-reactive) transport along with an in-depth interpretation of the MRF theory should improve the depiction of such temporal variability in our models.

What are the basic errors in biogeochemical models?

In the past decades, profound advances have been made in our understanding of the transport of reactive chemicals in natural porous media such as soil and aquifers. Aside from the specialized models aimed at solving one particular physico-chemical problem (Tinker and Nye, 2000), generic tools with a broader application domain have also been constructed. Characteristic examples are the well-known packages of RT3D, PHREEQC, and ORCHESTRA (Parkhurst and Appelo, 1999; Meeussen, 2003). Of special interest is that such packages can be linked with multidimensional flow models, for example, to study processes in the rhizosphere (Szegedi *et al.*, 2008), or with heterogeneous flow domains (Wriedt and Rode, 2006). Yet, despite these significant improvements, several basic issues have remained unresolved. First, the chemical submodels are often formulated on a logarithmic scale of ion activities, and therefore reaction coefficients are expressed as

pK values ($-\log[K]$). In the rather non-idealized, non-pure earth systems, we rarely deal with pure crystals, salts, and minerals. Hence, if pK values are incorrect or flawed, as in the case of Meeussen (1992), this may lead to considerable errors (over an order of magnitude) in the original scale. Obviously, the ramifications on the calculated retardation factors can be quite substantial. Second, the assumption that local process descriptions hold at larger scales is at least questionable. In the context of reacting chemicals transport, this issue has been considered by pore network models of Acharya *et al.* (2005) and randomly heterogeneous aquifer of Janssen *et al.* (2006). As a first approximation, the transport of chemicals that undergo biogeochemical interactions is modelled by the incorporation of a reaction term in the well-known convection dispersion equation (CDE). The biogeochemical interaction term can be either linear or non-linear with regards to the chemical concentration. In the latter case, the solution of the CDE leads (for appropriate initial and boundary conditions) to the travelling wave (TW) type of displacement (Van der Zee, 1990; Van Duijn and Knabner, 1992). Both Acharya *et al.* (2005) and Janssen *et al.* (2006) modelled a porous medium that is characterized by spatial variability at a larger scale than that of discretization. As has been shown by Cirpka *et al.* (1999), the discretization of the flow domain, in case of non-linear reactions and spatial variability, requires special care, to avoid numerical dispersion problems. For example, Janssen *et al.* (2006) adopted a simplified biodegradation case with Monod kinetics to obtain a streamline adjusted discretization of their randomly heterogeneous domain which then enabled meaningful computations. As is shown (Figure 3) for an electron acceptor that enters the 2D flow domain from the left, this leads to an irregularly shaped domain. The initially present organic contaminant (blue area; concentrations are appropriately made dimensionless: Janssen *et al.*, 2006) is being degraded upon the introduction of the electron acceptor and the growth of the microbial mass that is responsible for the degradation, at the interface of the blue and red areas of Figure 3. The resulting pattern is strongly affected by both the spatial variability and the distinct non-linearity of the Monod-biomass growth affected degradation process. Using moment analysis, Janssen *et al.* (2006) showed for situations as depicted in Figure 3 that depending on the scales of the heterogeneity and of the dispersional mixing regimes considered, either heterogeneity or non-linear chemistry may dominate the transport behaviour.

It should be emphasized that major implications arise when attributing non-linear interactions to discrete volumes of arbitrary scale (often chosen for computational speed). In particular, if heterogeneity dominates, the non-linear transport is expected to approach the Fickian regime with a macrodispersivity that is affected by variance and correlation length of the heterogeneous field (Dagan, 1989). However, the latter regime is not the case, if transversal mixing dominates and the associated dispersivity is larger than the correlation length perpendicular to the mean flow. The transversal mixing 'homogenizes' the heterogeneous medium and, under appropriate conditions, TWs may develop (Van der Zee, 1990; Van Duijn and Knabner, 1992). Only in the latter case, it may be appropriate to use the CDE with a non-linear reaction term at the scale of discretization. A similar message was conveyed by Acharya *et al.* (2005) on the basis of pore network models. As non-linear biogeochemical models are never derived from empirical studies on samples of many cubic metres of porous media (and if they are, such samples are 'shaken' instead of undisturbed as in flow and transport models), it is quite questionable whether it is acceptable to combine non-linear biogeochemistry with any transport model with discretizations exceeding the level of several millimetres. Yet, the majority of our models are still based on such simplified approximations. Both examples discussed in this section imply that the local-scale descriptions should not be oversimplified, if we strive to maintain the correct behaviour at the larger scales. In both cases, it is emphasized that local process understanding needs to be related mechanistically with larger scale approaches.

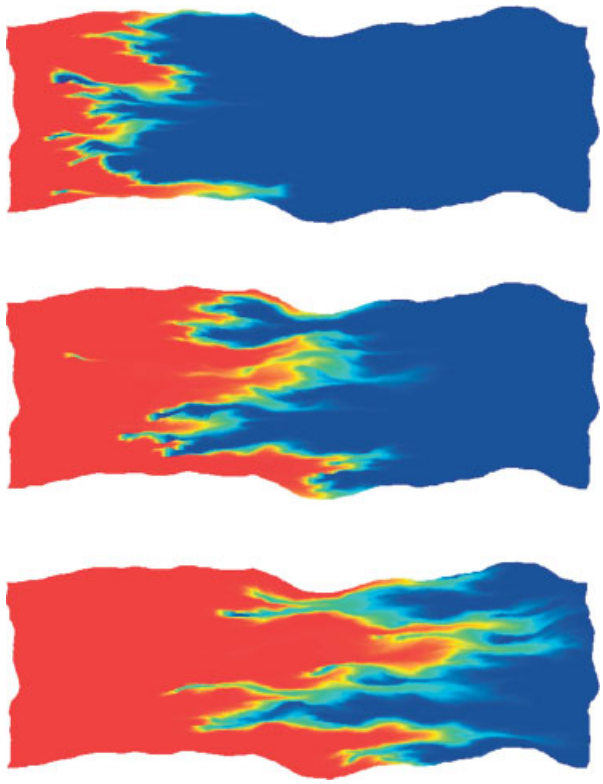

Figure 3. Three snapshots of solute transport for a random, exponentially autocorrelated hydraulic conductivity in an aquifer. The model assumes non-linear Monod biodegradation kinetics and a mixing zone affected by both the highly non-linear degradation interactions and pore-scale dispersion in a flow domain with spatial variability at a larger scale than that of pore-scale dispersion (Courtesy: Gijs Janssen, Wageningen University and Deltares, the Netherlands, 2006)

How can we define the appropriate complexity for process-based models at the regional scale?

The continuous dynamic regional river basin models are founded upon mathematical descriptions of physical, biogeochemical, and hydrochemical processes and

therefore can be called process-based ecohydrological (or water quality) models. These models combine significant elements of both physical and conceptual semi-empirical nature, containing reasonable spatial disaggregation schemes [e.g. subbasins and hydrologic response units (HRUs)], and may also include some stochastic elements. Characteristic examples of process-based modelling tools for river basins are the models SWAT (Arnold *et al*., 1994), HSPF (Bicknell *et al*., 2001), SWIM (Krysanova *et al*., 1998), and DWSM (Borah *et al*., 2004). Numerous studies published during the last decades have demonstrated that such models are able to adequately represent hydrological, biogeochemical, and vegetation growth processes at the catchment scale. However, the experience of using complex process-based models has also led to the conclusion that the model complexity should not be a self-purpose, and that the following rule has to be adopted by the model developers: if a complex natural phenomenon or process can be described mathematically in a simplified form and properly parameterized by the available data, this should be preferable to one with a higher level of details but also with higher number of unconstrained parameters. In the latter case, the model parameterization becomes problematic, and the control of the model behaviour may be difficult or impossible. In other words, one should include submodels that are essential, parameters that can be identified, and interrelations that can be understood and validated in simulation experiments.

Spatially distributed or semi-distributed models are usually required for improving the representation of biogeochemical processes while accommodating landscape heterogeneity. The simplest way to alleviate the lumped structure of a model is to subdivide a catchment into subcatchments or subbasins. This procedure enables to take into account differences in topography, soil types, or land use patterns in parts of the catchment, and also to consider spatial variations in model variables and parameters. Further subdivision of the land surface delineated by subbasins is possible using the principle of similarity. Usually for that the subbasin map, land use, and soil maps are overlaid to create the so-called hydrotopes or HRUs, which could be also combined into hydrotope classes within subbasins. Then a typical disaggregation scheme can be implemented in a model as a three-level process consisting of (i) the simulation of all the processes in the HRUs or hydrotopes, (ii) the aggregation of lateral flows in subbasins, and (iii) the routing of water, sediments, and dissolved matter over the entire catchment, while describing lateral transport of water, nutrients, and pollutants in some reasonable way.

The spatial and temporal resolution of the model is typically connected with the scale of the application and objective of the study, but should also be commensurate to the data availability. A fine spatial resolution may be required for a small catchment in order to study water flow components and their pathways using tracers. On the other hand, a lumped model may be sufficient for the case where the 'precipitation–runoff' relationships are only investigated in a homogeneous small or medium-size catchment. In a similar manner, a coarser resolution could be applied for mesoscale or large river basins for water resource assessments and climate impact studies where no detailed evaluation of management options is needed. Although attempts have been made to give guidance in reducing overall model uncertainties in environmental modelling (Refsgaard *et al*., 2007), a general framework for selecting the appropriate process and spatial model complexity for a given catchment is still missing.

Do we have suitable calibration datasets for complex distributed models?

Increasing spatial model complexity does not always improve model results. A case study using the SWIM model for simulating nitrogen loads in the large Saale catchment (Germany) showed that the use of distributed parameters for simulating nitrogen retention in the subsurface and groundwater during the transport of nitrogen from the soil column to the river network did not improve the results compared to the use of global retention parameters (Huang *et al*., 2009). The Saale is the second largest tributary of the Elbe river with the length of 427 km and the catchment area of 24·167 km^2 (FGG-Elbe, 2004). Wide loess areas and low mountain ranges characterize the catchment. Due to very fertile loess soils, more than two-thirds of the catchment area is used for agriculture. The term 'retention' in the model mainly encompasses soil and groundwater denitrification (see description of the approach in Hattermann *et al*., 2006).

The model validation for the whole Saale with the global retention parameters (Figure 4, upper graph) was quite satisfactory, with the Nash and Sutcliffe efficiency of 0·7. The hypothesis was that the use of distributed retention parameters could improve the validation results in the intermediate (not calibrated) gauges. The set-up of simulation experiments and results are described in detail in Huang *et al*. (2009). In fact, the results for distributed parameter settings, which were based on different denitrification conditions specified by Wendland *et al*. (1993), were very similar to those derived from the global parameterization (Figure 4, lower graph), and the model fit for some intermediate gauges was even worse under the distributed parameter setting. It was hypothesized that this counterintuitive result primarily stemmed from the uncertainties in estimated soil and groundwater denitrification conditions, as karstic areas within the basin may affect denitrification conditions. Hence, the data on groundwater properties were insufficient to conduct a highly distributed calibration and this example pinpoints the importance of the data availability problem for the reliability of distributed catchment models. Future work should therefore focus on how and to what extent improved data availability could enhance the model quality in terms of the representation of the observed nutrient dynamics. Critical model evaluation (e.g. using Bayesian calibration frameworks) can be used to determine the

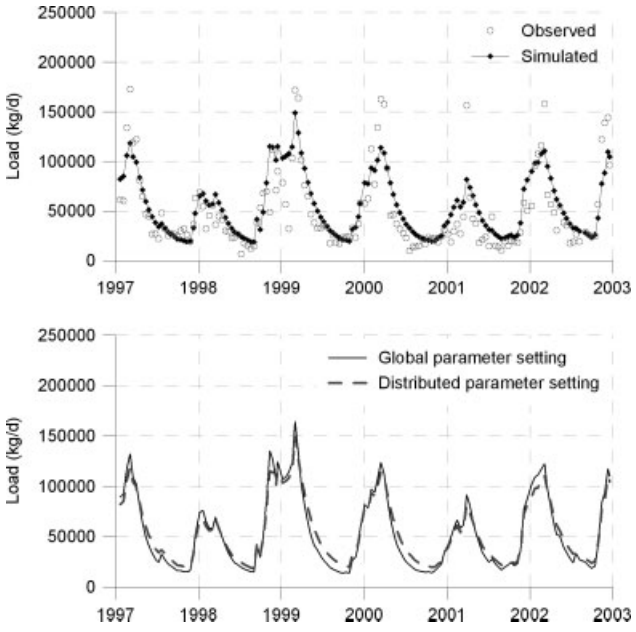

Figure 4. Validation of nitrogen load dynamics for the Saale basin, gauge Gross–Rosenburg (upper graph), and comparison of simulations for the same gauge station with the global and distributed retention parameter settings (lower graph) (Huang *et al*., 2009)

optimal sampling design and to assess the value of information contained by the data (Rode *et al*., 2007, Zhang and Arhonditsis, 2008).

IN-STREAM NUTRIENT TRANSPORT MODELLING

In-stream mass transformation is controlled by various processes in different compartments (pelagic, river bed, and hyporheic zones) with varying importance as we move from the headwaters to the mid-reach streams and finally to the downstream regions (Borchardt and Pusch, 2009). Large rivers are more likely to be dominated by transport and conversion processes in the pelagic zone. In contrast, headwater streams and mid-stream regions with coarse substrates are affected by both resuspension processes and benthic activity as well as the hyporheic zone effects. Recent studies suggest that the hyporheic zone plays an important role in maintaining and regulating in-stream nutrient metabolism (Jones and Mulholland, 2000; Birgand *et al*., 2007; Ingendahl *et al*., 2009).

Do we place sufficient emphasis on hyporheic processes?

The hyporheic zone may be loosely defined as the porous areas of the stream bed and stream bank where the stream water mixes with shallow groundwater. Due to the differences in chemical composition of the surface water and groundwater, exchange of water and solute between stream and hyporheic zone have many biogeochemical implications (Runkel *et al*., 2003). Hyporheic zones influence the biogeochemistry of stream ecosystems by increasing solute residence times; specifically, the contact of solutes with substrates increases in environments with pronounced dissolved oxygen and pH spatial gradients (Bencala, 2000). The influence of hyporheic exchange upon the transport and transformation of solutes occurs in environments where hydrologic and biogeochemical processes are dynamic and highly heterogeneous. Documenting the biogeochemical function of the hyporheic exchange has thus been primarily accomplished in high sampling intensity research (Bencala, 2005). Aside from the nutrient (P, N) conversion, the hydrological exchange between the river and its hyporheic zone has also a strong influence on the fauna distribution, the transport of organic matter, and the metabolism in the hyporheic zone (Pusch, 1996; Naegeli and Uehlinger, 1997).

Water quality models are often implemented in order to quantify the substance transformation in lotic waters and to investigate the impact of changes of the boundary conditions on aquatic ecosystem dynamics. Most conventional river water quality models (e.g. QUAL2E, WASP5, Mike 11) focus on biological processes in which nutrient decomposition is considered as a first order decay process without explicitly accounting for the role of the hyporheic zone processes, for example, denitrification (Wagenschein and Rode, 2008). Although improved process-oriented approaches for explicitly describing nutrient transformations in the hyporheic zone have been developed (Reichert *et al*., 2001; Sheibley *et al*., 2003; Runkel, 2007), their application is still problematic because site-specific data are often sparse, and parameters of hydraulic equations or biogeochemical rate constants are often unknown. Future research should specifically focus on the elucidation of the importance of the water column-hyporheic zone interactions as well as on the role of advective exchanges in modulating the nutrient metabolism. Variables such as hydraulic conductivity, grain size distribution, stream bed geometry, and stream velocity are critical measurement requirements (Findlay, 1995; Birgand *et al*., 2007).

Do biological processes play an important role on hyporheic exchange?

Water exchange between hyporheic zone and the water column are not exclusively controlled by physical properties. New findings showed that biological processes may also have significant impact on this advective exchange. Ibisch *et al*. (2006) reported a clear negative exponential relationship between infiltration rates and periphyton biomass. The same study concluded that external colmation by periphyton is an important process in eutrophic rivers controlling hyporheic exchange patterns. Decolmation is the reverse process of colmation, that is the loosening of compacted structures and the return to a state with higher sediment permeability (Schälchli, 1993). This decolmation is not only induced by physical processes (Sengschmitt *et al*., 1999), as biogenic decolmation due to bioturbation of the interstitial fauna may also increase the permeability of the sediment matrix (Findlay, 1995; Ward *et al*., 1998; Hakenkamp and Morin, 2000; Mermillod-Blondin *et al*., 2000). A recent study by Schmidt *et al*. (2009) showed that bioturbation and grazing activities by meiofauna have a measurable impact

on the permeability of the stream sediments. These findings may offer new insights into the functional role of interstitial fauna for the self-purification of polluted river sections. The quantification of the relative role of physical and biological processes on the water column-hyporheic zone exchanges constitutes a challenge for future ecological research.

How can we improve regional scale in-stream nutrient transport modelling?

The uncertainties in simulating natural in-stream attenuation processes at the local scale are magnified when undertaking predictions of nutrient transport and attenuation processes across various stream network characteristics (Darracq and Destouni, 2007). Most contemporary operational models of in-stream nutrient transport use simple empirical relationships, which are based on statistical analysis of large data sets (Alexander *et al*., 2000, 2009; Behrendt and Opitz, 2000; de Wit, 2001). New findings provide evidence that transformation processes are highly non-linear, which implies that the simple empirical relationships have limited capacity for predicting unknown future states with variable nutrient concentrations or climate conditions (Mulholland *et al*., 2008). Furthermore, there is an ongoing debate on the scaling of nutrient removal from small streams up to larger river sizes (Alexander *et al*., 2006; Destouni and Darracq, 2006; Wollheim *et al*., 2006). Because most process-based studies on in-stream nutrient attenuation focus on small headwater streams, we propose scale-dependent studies which cover the full range of stream/river scales and give special consideration on the hyporheic zone. Currently, process-based nutrient transport research especially in mid-river scales is sparse (Mulholland *et al*., 2008). If most important river types and network characteristics are covered, it should be possible to develop process-based models with higher predictive capabilities. Additional knowledge on detailed physical transport processes can be provided by non-reactive tracer studies where novel mobile aquatic mesocosm approaches, offering reasonable approximations to natural surface waters, may allow insights into the biogeochemical processes influencing in-stream nutrient turnover (Battin *et al*., 2003; Evans-White and Lamberti, 2005; Petersen and Englund, 2005).

LINKAGE OF CATCHMENT AND RECEIVING WATER BODY MODELS

The coupling of catchment with in-stream processes raises several practical problems with regards to the typical spatiotemporal resolution mismatch among the different submodels, the propagation of uncertainty through the complex model structures derived from the combination of the individual components, the integration of the different modules with an easy, flexible, and transparent way, and the uniqueness of some local processes that hamper the development of a general protocol for assembling the submodels into one coherent framework.

What is the appropriate model linkage strategy?

Only few attempts have been made to fully couple distributed catchment models with complex river water quality models. This coupling can be done at different levels. A distinction can be made between external linking, through file exchange, and internal linking, through the internal computer memory. External file exchange often requires programming (reformatting) or intensive labour as there is no standardized format for model input/outputs. The alternative linking, through memory, is adopted in several forms. The tight integration is known by the MIKE-SHE modelling software, whereby the distributed catchment model SHE is fully integrated towards the dynamic river model, known as Mike11 (Graham and Butts, 2006). The latter tool is easily applicable and computationally efficient but lacks flexibility to link up to other tools or processes.

Another form of integration is done by developing modular structures within a certain framework, for example, the Java-based Modular Modelling System (Leavesley *et al*., 2006) and the Object Modelling System (Kralisch *et al*., 2005, Rode *et al*., 2009, Hesser *et al*., 2010). A third option is integrating different software packages into a single framework. In the United States, the framework for risk analysis in multimedia environmental systems—multimedia, multipathway, and multireceptor risk assessment (FRAMES-3MRA)—is an important model being developed by the United States Environmental Protection Agency for risk assessment of hazardous waste management facilities (Babendreier and Castleton, 2008). In Europe, the OpenMI interface aims at integrating independent modelling software, after being slightly modified as OpenMI compliant versions, in order to be applied within a common interface that manages the simulations of the submodels at running time and the exchange of model outputs (Gregersen *et al*., 2007). There is little additional computation time by the functioning of the interface as long as not too many software applications or dynamic links are involved (e.g. 1D-2D integration). A characteristic example is the work by Getnet (2009), who used OpenMI to link a catchment model (soil and water assessment tool) to a river model (SOBEK) for simulating erosion and sediment transport processes.

How can we ensure transparency of complex integrated models?

In addition to flexibility, transparency is a key word. A good integrated modelling practice is a decentralized one, whereby the subsystems are individually calibrated and validated as much as possible. Whatever format is adopted for model integration, it leads undoubtedly to higher complexity and higher uncertainty. Furthermore, the complexity of submodels often differs significantly which creates problems in model linkage or imbalanced process description with regard to their importance for water and mass transport. For example, many distributed catchment models place emphasis on detailed soil process

description but use very simple lumped descriptions for groundwater transport and biogeochemistry (e.g. SWAT, HSPF). The latter issue can be perceived as another aspect of the 'change of support' problem (sensu Wikle, 2003), and has received considerable attention in the modelling literature (Wikle and Berliner, 2005; see also following section).

The application of the coupled catchment-receiving water body modelling constructs involves substantial uncertainty contributed by both model structure and parameters. One of the future challenges is to develop calibration frameworks that assess the effects and propagation of uncertainty in integrated environmental modelling systems, allow insights into the degree of information the data contain about model inputs, and effectively link land use changes in the watershed (e.g. urbanization) with the responses of the receiving waterbody (e.g. Vandenberghe *et al*., 2002). A screening of the different sources of uncertainty has been attempted by efficient sampling designs such as the Latin-Hypercube sampling or the One-Factor-at-a-Time design (Vandenberghe *et al*., 2001; Van Griensven *et al*., 2006). Furthermore, model structure can be evaluated by ensemble modelling (e.g. McIntyre *et al*., 2005; Viney *et al*., 2005). Integrating the results of a number of candidate model structures, rather than simply assuming one model structure, may significantly reduce prediction bias and enhance model transparency (Neuman, 2003).

UNCERTAINTIES IN WATER QUALITY MODELLING

As the articulation level of our water quality models continues to grow, an emerging imperative is the development of novel uncertainty analysis techniques to rigorously assess the error pertaining to model structure and input parameters (Reichert and Omlin, 1997). The assessment of the uncertainty characterizing the multidimensional parameter spaces of mathematical models involves two important decisions: (i) selection of the likelihood measure to quantify model error and (ii) selection of the sampling algorithms to generate a series of model realizations. Arhonditsis *et al*. (2007) has recently introduced a Bayesian calibration methodology founded upon Markov chain Monte Carlo (MCMC) sampling schemes and Gaussian likelihoods that can explicitly accommodate measurement error, parameter uncertainty, and model structure imperfection. Avoiding overly complex model constructs, the proposed framework combines the advantageous features of both process-based and statistical approaches in that the models offer mechanistic understanding but still remain within the bounds of data-based parameter estimation. The incorporation of mechanism improves the confidence in predictions made for a variety of conditions, while the statistical methods provide an empirical basis for parameter estimation. In a subsequent study, Zhang and Arhonditsis (2008) have illustrated some of the benefits for environmental management from the Bayesian calibration framework, such as the assessment of the exceedance frequency and confidence of compliance with different water quality criteria, probabilistic inference on cause-effect relationships pertaining to water quality management, optimization of monitoring programs using value of information concepts from decision theory, and alignment with the policy practice of adaptive management implementation.

Yet, several technical issues regarding the formulation of the error structure, the selection of the parameter priors and likelihood functions, the optimal model complexity, and the computational efficiency of the Bayesian calibration scheme require particular attention and/or invite further investigation.

How can we distinguish among different sources of uncertainty?

The uncertainty in water quality modelling generally stems from several sources of error: input and response uncertainty, that is errors associated with measurements of input (rainfall) and response data, such as water level, flow discharge, water quality variables (Rode and Suhr, 2007), parametric uncertainty, and structural error arising from the intrinsic inability of a given model structure to reproduce the mechanisms involved in runoff generation or in biogeochemistry (Montanari, 2004). Bayesian theory coupled with MCMC sampling strategies has proven to be a valuable means for evaluating the effects of the different sources of uncertainty in simple lumped as well as in more complex fully distributed hydrological models (Kavetski *et al*., 2002, 2006; Balin, 2004; Ajami *et al*., 2007; Huard and Mailhot, 2006; Marshall *et al*., 2006). Balin *et al*. (2010) presented a Bayesian approach for assessing the impact of errors of input rainfall data on distributed hydrological modelling (Balin, 2004). The characterization of the rainfall data error was modelled with a hierarchical normal model, where the first level of hierarchy specified the measurement error for the observed noisy data which then were associated with the true unknown rainfall data. This model configuration, however, did not lead to substantially different results with regards to the estimated parameters, model efficiency, and uncertainty of the simulated water discharges (Balin *et al*., 2010). The latter finding may be due to the fact that other sources of uncertainty contribute more to the total uncertainty of distributed hydrological modelling rather than the point random measurement error in the rainfall data. Interestingly, when the spatial rainfall uncertainty was taken into account by means of rainfall conditional simulations using the Turning Band Algorithm, the same modelling exercise showed that the impact of the underlying uncertainty on both estimated parameters and predicted responses was substantially more important (Balin *et al*., 2010). Without any intent of generalizing, this example indicates that the scientists should be careful when attempting to associate the different sources of uncertainty with the predictions provided by environmental models. There is an urgent

need to explore the role of different sources of uncertainty in hydrological and water quality models and to improve their use for operational and decisional purposes by developing novel uncertainty analysis methodological frameworks (Kuczera and Parent, 1998; Kavetski *et al*., 2002, 2006; Balin, 2004; Marshall *et al*., 2006; Ajami *et al*., 2007; Yang *et al*., 2007).

How can we improve the assessment of model structural errors?

The statistical representation of the model error can significantly alter the inference about the parameter posteriors as well as the model predictive distributions (Thiemann *et al*., 2001). Arhonditsis *et al*. (2008) noted that statistical formulations that postulate a 'perfect' model structure and a model misfit solely caused by the data error tend to provide narrow-shaped parameter distributions. This result, however, does not necessarily depict the amount of knowledge gained with regards to the parameter values when considering prior literature information and available data from the system modelled, and may be attributed to an overconditioning of the parameter estimates owing to an overestimation of the information content of the observations. By contrast, statistical formulations that explicitly consider errors in the model specification (e.g. missing key ecological processes, misspecified forcing functions, erroneous formulations) improve model performance, although the parameter posteriors tend to be flatter (Higdon *et al*., 2004; Arhonditsis *et al*., 2008). The development of statistical formulations explicitly recognizing the lack of perfect simulators of natural system dynamics is a promising prospect for the Bayesian calibration framework, and future research should also accommodate the spatiotemporal dependence patterns of the parameter values and model error terms.

How can we balance robustness of uncertainty analysis and associated computational demands?

Robust Bayesian analysis is a promising framework to rigorously assess the conclusions drawn from typical uncertainty analysis applications based on single prior distributions and/or likelihood functions (Berger, 1994). For example, Tomassini *et al*. (2007) examined the robustness of the uncertainty analysis results of climate system properties using classes of parameter priors, different scaling of the observational error, and alternative likelihood functions. The posterior predictive patterns highlighted the critical role of the prior parameter distributions, and also dictated areas where future data collection efforts should focus on to constrain climate model sensitivity. Despite its sound premise though, the potential for broad adoption of robust Bayesian uncertainty analysis in water quality modelling is still unclear given the computational demands that this framework entails.

Recent efforts to improve the computational efficiency of MCMC implementations of Bayesian inference for water quality models focussed on the development of parallel algorithms (Altekar *et al*., 2004; Whiley and Wilson, 2004). Parallel computation for MCMC can reduce the time needed to generate a sufficient number of samples from target distributions of larger dimensions, although Whiley and Wilson (2004) assert that a good proposal distribution is of equal importance as the implementation of a parallelization scheme. Alternatively, Higdon *et al*. (2004) proposed a compromise between the 'fidelity of the simulator' and the 'simulation speed' claiming that a comprehensive examination of the posterior distribution of a simple model can be more informative than an insufficient posterior approximation of a more complex model. Moreover, additional model complexity does not necessarily imply more MCMC runs; if the number of parameters that drive the model outputs does not change, then the number of runs required to sufficiently approximate the posterior will not be significantly different (Jansen and Hagenaars, 2004). In the modelling practice, our experience is also that only a subset of the input parameters is influential on the outputs of water quality models (Omlin *et al*., 2001; Arhonditsis and Brett, 2005), and therefore an effective calibration does not always require statistical formulations framed in a hyperdimensional context (Kennedy and O'Hagan, 2001).

How can we define the optimal model complexity?

The latter point also raises the issue of the optimal model complexity selection. Zhang and Arhonditsis (2008) emphasized that the integration of the Bayesian calibration framework with complex overparameterized simulation models disallows meaningful insights into the ecosystem functioning (e.g. realistic magnitudes of the various ecological processes), despite the satisfactory fit to the observed data that is usually obtained. Acknowledging the increasing demand for complex water quality models in the contemporary modelling practice, the same study suggested that the rigid structure of complex mathematical models can be replaced by more flexible modelling tools (e.g. Bayesian networks) with the ability to integrate quantitative descriptions of ecological processes at multiple scales and in a variety of forms (intermediate complexity mathematical models, empirical equations, expert judgements), depending on available information (Borsuk *et al*., 2004). Other interesting ideas in the literature include strategies for dimension reduction, adaptive designs to overcome limited number of simulation runs, and replacement of the simulators with statistical models that encompass key features of the modelled system (Craig *et al*., 2001; Goldstein and Rougier, 2004; Higdon *et al*., 2004).

The Bayesian paradigm has also been considered as a means for addressing the different issues that fall under the 'change of support' topic (Wikle, 2003). In particular, Bayesian approaches have been used to alleviate problems of spatiotemporal resolution mismatch among different submodels of integrated environmental modelling systems, to overcome the conceptual or scale misalignment between processes of interest and

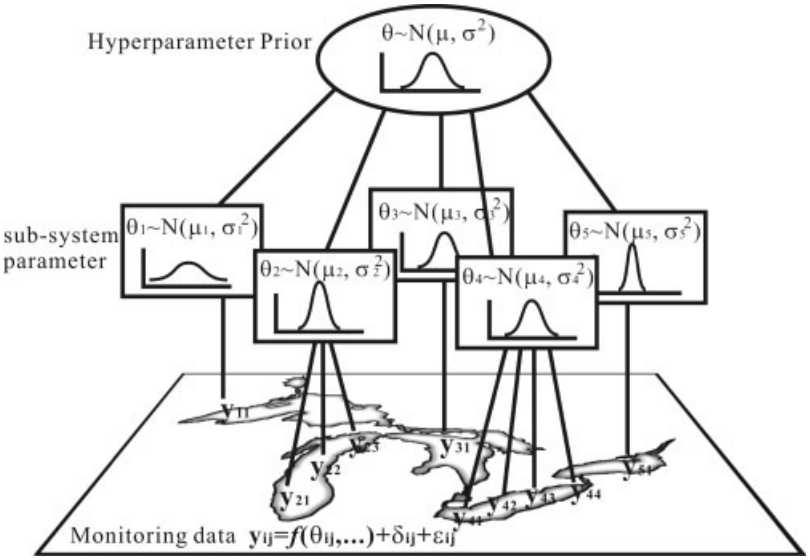

Figure 5. A conceptual application of the Bayesian hierarchical framework to allow the transfer of information in space (Zhang and Arhonditsis, 2009)

supporting information, to exploit disparate sources of information that differ with regards to the measurement error and resolution, to accommodate tightly intertwined environmental processes operating at different spatiotemporal scales, and to explicitly consider the variability pertaining to latent variables or other inherently 'unmeasurable' quantities. The existing propositions involve general hierarchical spatial model frameworks (Cressie, 2000; Wikle *et al*., 2001; Wikle, 2003), Markov random field models (Besag *et al*., 1995), and hierarchical spatiotemporal models that are simplified by dimension reduction (Berliner *et al*., 2000) or by conditioning on processes considered to be latent or hidden (Hughes and Guttorp, 1994). In the same general context, Zhang and Arhonditsis (2009) advocated the relaxation of the assumption of globally common parameter values used in coupled physical-biogeochemical process-based models and the adoption of hierarchical statistical formulations that reflect the more realistic notion that each site is unique but shares some commonality of behaviour with other sites of the same system. The proposed approach represents a practical compromise between entirely site-specific and globally common parameter estimates and may be a conceptually more sound strategy to accommodate the spatial variability observed in terrestrial as well as in aquatic ecosystems. A conceptual application of the Bayesian hierarchical framework to allow the transfer of information in space is shown in Figure 5. The problem of parameter estimation is viewed as a hierarchy. At the bottom of the hierarchy are the process-based models for individual waterbodies i and sites j, $f(\theta_{ij})$. In the next level, the spatial heterogeneity is accommodated by introducing $i(=5)$ lake-specific or 'regional' distributions; that is depending on the lake that the individual sites belong, the model parameters θ_{ij} are drawn from one of these local populations. Similarly, in the upper stage, the local population parameters μ_i and σ_i are specified probabilistically in terms of global population parameters or hyper-parameters; for example, a global mean μ and variance σ that correspond to the wider Great Lakes area. The observed data y_{ij} are used to estimate the model parameters θ_{ij}, the 'regional' population parameters μ_i, σ_j and the hyper-parameters μ, σ. The terms δ_{ij} and ε_{ij} represent the site-specific structural and measurement errors, respectively (Zhang and Arhonditsis, 2009).

CONCLUSIONS

One of the fundamental problems on catchment-scale water quality modelling is that the integration of non-linear biogeochemistry with any transport model may lead to considerable uncertainty, because the study scale for deriving the reaction terms differs significantly from the model application scale. Considerable errors may also arise from the use of logarithmic scales. Therefore, we propose the following.

1. Simpler linear models should be used at larger scales, if the rigorous evaluation of non-linear biogeochemical models is not possible at the application scale.
2. Because the upscaling of process knowledge in catchment-scale modelling is still an unresolved problem, we advocate a shift in the focus of combined field and modelling process-based studies. Namely, scale-dependent process studies which systematically cover the entire range of river scales and catchment characteristics is very likely to bolster the predictive capacity of process-based models at larger scales.
3. Research priorities and selection of representative sites should be driven by the importance of a given transport phenomenon for the water quality at the catchment scale of interest. Our current understanding, for example, suggests that groundwater/surface water interactions are scale dependent and may become less significant with increasing stream order.
4. The spatial and temporal resolution as well as the model complexity should always be related to the scale

of application, the objective of the study, the knowledge on the key processes, and the data availability.

Compared to terrestrial ecosystems, we think that the importance of in-stream nutrient (mainly phosphorus and nitrogen) transport processes is not adequately represented in most integrated water quality models. Most conventional river water quality models do not explicitly account for the role of hyporheic zone processes. Therefore, we suggest the following.

1. Future research should specifically focus on improving our understanding and mathematical description of the water column-hyporheic zone interactions as well as the role of advective exchanges on nutrient metabolism.
2. Bioturbation and grazing activities by meiofauna impact the permeability of stream sediments. Therefore, the quantification of the relative role of physical and biological processes on the water column-hyporheic zone exchange constitutes a challenge for future ecological research.
3. We propose scale-dependent studies on in-stream nutrient attenuation processes which cover the full range of stream/river scales and give special consideration on the hyporheic zone.
4. Novel mobile aquatic mesocosm approaches may allow insights into biogeochemical processes influencing in-stream nutrient turnover.

Coupling of catchment with in-stream process raises several practical problems which are closely related to uncertainty assessment of integrated water quality models, especially to model structure and input parameters.

1. We found that the integration through new software such as OpenMI or through modular structures offers promising prospects to effectively couple quantitative descriptions of ecological processes at multiple scales.
2. Keeping the growing complexity of integrated water quality models in mind, the development of novel uncertainty analysis techniques for rigorous assessing parameter identification and model credibility is essential.
3. We recommend the use of Bayesian calibration frameworks that explicitly accommodate the measurement errors, parameter uncertainties, and model structure errors. The Bayesian inference can be used to quantify the information the data contain about model inputs, to offer insights into the covariance structure among parameter estimates, to obtain predictions along with credible intervals for model outputs, and to effectively address the 'change of support' problems.
4. To overcome the computation demands of MCMC implementations of Bayesian inference for integrated water quality models, recent promising efforts involve the development of adaptive sampling algorithms and parallel computing schemes.

Despite all the uncertainties associated with limited input data, water quality models are increasingly important tools to support water managers and policy makers in implementing integrated water resources management (IWRM). It would be impossible to evaluate the effectiveness of alternative watershed management plans (e.g. land use changes) or the repercussions of climate change on water quality without using modelling tools. The dynamic catchment models include water and nutrient processes as a function of the vegetation, climate, and human impacts, thereby offering a useful methodology for projecting future system responses and for designing river basin management plans accordingly. The improvement of our mechanistic understanding at multiple scales along with development of novel methods for accommodating rigorous and complete error analysis are the imperative challenges for the future of integrated water quality modelling.

REFERENCES

Acharya RC, van der Zee SEATM, Leijnse A. 2005. Transport modeling of nonlinearly adsorbing solutes in physically heterogeneous pore networks. *Water Resources Research* **41**: W02020. DOI: 10.1029/2004WR003500.

Ajami N, Duan KQ, Sorooshian S. 2007. An integrated hydrologic Bayesian multimodel combination framework: confronting input, parameter, and model structural uncertainty in hydrologic prediction. *Water Resources Research* **43**: W01403.

Alexander RB, Smith RA, Schwarz GE. 2000. Effect of stream channel size on the delivery of nitrogen to the Gulf of Mexico. *Nature* **403**: 758.

Alexander RB, Smith RA, Schwarz GE. 2006. Comment on "In-stream nitrogen attenuation: model-aggregation effects and implications for coastal nitrogen impacts". *Environmental Science and Technology* **40**: 2485–2486.

Alexander RB, Böhlke JK, Boyer EW, David MB, Harvey JW, Mulholland PJ, Seitzinger SP, Tobias CR, Tonitto C, Wollheim WM. 2009. Dynamic modeling of nitrogen losses in river networks unravels the coupled effects of hydrological and biogeochemical processes. *Biogeochemistry* **93**: 91–116.

Altekar G, Dwarkadas S, Huelsenbeck JP, Ronquist F. 2004. Parallel metropolis coupled Markov chain Monte Carlo for Bayesian phylogenetic inference. *Bioinformatics* **20**: 407–415.

Arhonditsis GB, Brett MT. 2005. Eutrophication model for Lake Washington (USA) Part I—model description and sensitivity analysis. *Ecological Modeling* **187**(2–3): 140–178.

Arhonditsis G, Giourga C, Loumou A, Koulouri M. 2002. Quantitative assessment of agricultural runoff and soil erosion using mathematical modelling: applications in the Mediterranean region. *Environmental Management* **30**: 434–453.

Arhonditsis GB, Adams-Vanharn BA, Nielsen L, Stow CA, Reckhow KH. 2006. Evaluation of current state of mechanistic aquatic biogeochemical modeling: citation analysis and future perspectives. *Environmental Science and Technology* **40**: 6547–6554.

Arhonditsis GB, Qian SS, Stow CA, Lamon EC, Reckhow KH. 2007. Eutrophication risk assessment using Bayesian calibration of process-based models: application to a mesotrophic lake. *Ecological Modeling* **208**(2–4): 215–229.

Arhonditsis GB, Perhar G, Zhang W, Massos E, Shi M, Das A. 2008. Addressing equifinality and uncertainty in eutrophication models. *Water Resources Research* **44**: W01420.

Arnold JG, Williams JR, Srinivasan R, King KW, Griggs RH. 1994. *Soil and Water Assessment Tool*, USDA, Agricultural Research Service, Grassland, Soil and Water Research Laboratory: Temple, TX 76502, USA.

Babendreier JE, Castleton KJ. 2008. Investigating uncertainty and sensitivity in integrated, multimedia environmental models: tools for FRAMES-3MRA. *Environmental Modeling and Software* **20**(8): 1043–1055.

Balin D. 2004. *Hydrological behavior through experimental and modeling approaches. Application to the Haute-Mentue catchment*, PhD Thesis, Ecole Polytechnique Federale de Lausanne, Thesis Nr 3007, Lausanne.

Balin D, Hyosang L, Rode M. 2010. Is uncertain rainfall likely to greatly impact on distributed complex hydrological modeling. *Water Resources Research* DOI: 10.1029/2009WR007848, in press.

Battin TJ, Kaplan LA, Newbold JD, Hansen CME. 2003. Contributions of microbial biofilms to ecosystem processes in stream mesocosms. *Nature* **426**: 439–442.

Beck MB. 1999. Coping with ever larger problems, models and data bases. *Water Science and Technology* **39**(4): 1–11.

Behrendt H, Opitz D. 2000. Retention of nutrients in river systems: dependence on specific runoff and hydraulic load. *Hydrobiologia* **410**: 111–122.

Bencala KE. 2000. Hyporheic zone hydrological processes. *Hydrological Processes* **14**: 2797–2798.

Bencala KE. 2005. Hyporheic exchange flows. *Encyclopedia of Hydrological Sciences*, J. Wiley: Chichester, England; Hoboken, NJ.

Berger J. 1994. An overview of robust Bayesian analysis. *Test* **3**: 5–124.

Berliner LM, Wikle CK, Cressie N. 2000. Long-lead prediction of Pacific SSTs via Bayesian dynamic modeling. *Journal Climate* **13**(22): 3953–3968.

Besag J, Green P, Higdon D, Mengersen K. 1995. Bayesian computation and stochastic systems. *Statistical Science* **10**(1): 3–66.

Beven KJ. 1993. Prophecy, reality and uncertainty in distributed hydrological modeling. *Advances in Water Resources* **6**: 41–51.

Beven KJ. 2006. A manifesto for the equifinality thesis. *Journal of Hydrology* **320**(1–2): 18–36.

Bicknell BR, Imhoff JC, Kittle JL, *Jr.*, Jobes and TH, Donigian AS, *Jr.*. 2001. *Hydrological Simulation Program—Fortran: HSPF Version 12 User's Manual*, U.S. Environmental Protection Agency: Athens, GA. www.epa.gov/waterscience/basins/bsnsdocs.html#hspf.

Birgand F, Skaggs RW, Chescheir GM, Gilliam JW. 2007. Nitrogen removal in streams of agricultural catchments—a literature review. *Critical Reviews in Environmental Science and Technology* **37**: 381–487.

Borah DK, Bera, M, Xia R. 2004. Storm event flow and sediment simulations in agricultural watersheds using DWSM. *Transactions of the ASAE* **47**(5): 1539–1559.

Borah DK, Yagow G, Saleh A, Barnes PL, Rosenthal W, Krug EC, Hauck LM. 2006. Sediment and nutrient modeling for TMDL development and implementation. *Transactions of the ASABE* **49**(4): 967–986.

Borchardt D, Pusch M. 2009. An integrative, interdisciplinary research approach for the identification of patterns, processes and bottleneck functions of the hyporheic zone of running waters. *Advances in Limnology* **61**: 1–7.

Borsuk ME, Stow CA, Reckhow KH. 2004. A Bayesian network of eutrophication models for synthesis, prediction, and uncertainty analysis. *Ecological Modeling* **173**(2–3): 219–239.

Bouraoui F, Grizzetti B, Adelskold G, Behrendt H, Fawcett L, Gomez S, Granlund K, Hoffmann L, Kronvang B, Kværnø S, Lazar A, Mimikou M, Passarella G, Panagos P, Reisser H, Schwarzl B, Siderius C, Sileika AS, Sugrue R, Van Liedekerke M, Zaloudık J. 2009. Basin characteristics and nutrient losses: the EUROHARP catchment network perspective. *Journal of Environmental Monitoring* **11**(3): 515–525.

Cirpka OA, Frind EO, Helmig R. 1999. Streamline-oriented grid generation for transport modeling in two-dimensional domains including wells. *Advances in Water Resources* **22**: 697–710.

Conley DJ, Paerl HW, Howarth RW, Boesch DF, Seitzinger SP, Havens KE, Lancelot C, Likens GE. 2009. ECOLOGY controlling eutrophication: nitrogen and phosphorus. *Science* **323**: 1014–1015.

Craig PS, Goldstein M, Rougier JC, Seheult AH. 2001. Bayesian forecasting for complex systems using computer simulators. *Journal of the American Statistical Association* **96**: 717–729.

Cressie N. 2000. Spatial statistics and environmental sciences. *Proceedings of the Section on Statistics and the Environment*, American Statistical Association: Alexandria; 1–10.

Dagan G. 1989. *Flow and Transport in Porous Formations*, Springer-Verlag: Heidelberg, Berlin, New York; 465.

Darracq A, Destouni G. 2005. In-stream nitrogen attenuation: model-aggregation effects and implications for coastal nitrogen impacts. *Environmental Science and Technology* DOI: 0.1021/es0497400.

Darracq A, Destouni G. 2007. Physical versus biogeochemical interpretations of nitrogen and phosphorus attenuation in streams and its dependence on stream characteristics. *Global Biogeochemical Cycles* **21**: 1–9.

De Louw PGB. 2007. Brakke kwel in diepe polders: Case Polder de Noordplas. In *Verzilting in Nederland. NHV-special 7. Verzilting in Nederland. Nederlandse Hydrologische Vereniging*. ISBN:10-90-803565-7-3 (in Dutch).

de Wit MJM. 2001. Nutrient fluxes at the river basin scale. Part I: the PolFlow model. *Hydrological Processes* **15**: 743–759.

Denman KL. 2003. Modeling planktonic ecosystems: parameterizing complexity. *Progress in Oceanography* **57**: 429–452.

Destouni G, Darracq A. 2006. Response to Comment on "In-stream nitrogen attenuation: model-aggregation effects and implications for coastal nitrogen impacts". *Environmental Science and Technology* **40**: 2487–2488.

Ebel BA, Loague K. 2006. Physics-based hydrologic-response simulation: seeing through the fog of equifinality. *Hydrological Processes* **20**(13): 2887–2900.

Evans-White MA, Lamberti GA. 2005. Grazer species effects on epilithon nutrient composition. *Freshwater Biology* **50**: 1853–1863.

Findlay S. 1995. Importance of surface-subsurface exchange in stream ecosystems: the hyporheic zone. *Limnology and Oceanography.* **40**: 159–164.

FGG-Elbe. 2004. *Berichtüber die Umsetzung der Anhänge II, III und IV der Richtlinie 2000/60/EG im Koordinierungsraum Saale (B-Bericht)*. Vorlage zur Elbe-Ministerkonferenz am 9. Dezember 2004 (http://fgg-elbe.de/joomla/index.php?option=com_content&task=view&id=28&lang=de).

Getnet DB. 2009. Integrated sediment transport modeling using SWAT-SOBEK OpenMI for Blue Nile. In *Proceedings of the Hydroinformatics Conference, Chile*.

Goldstein M, Rougier J. 2004. Probabilistic formulations for transferring inferences from mathematical models to physical systems. *SIAM Journal on Scientific Computing* **26**: 467–487.

Graham DN, Butts MB. 2006. In *Flexible, Integrated Watershed Modeling with MIKE SHE, Watershed Models*, Singh and VP, Frevert DK (eds). Water Resources Publication: Highlands Ranch, Colorado; 245–272.

Gregersen JB, Gijsbers PJA, Westen SJP. 2007. OpenMI: Open modeling interface. *Journal of Hydroinformatics* **9**: 175–191.

Hakenkamp CC, Morin A. 2000. The importance of meiofauna to lotic ecosystem functioning. *Freshwater Biology* **44**: 165–175.

Harvey JW, Saiers JE, Newlin JT. 2005. Solute transport and storage mechanisms in wetlands of the Everglades, south Florida. *Water Resources Research* **41**: W05009. DOI: 10.1029/2004WR003507.

Hattermann FF, Krysanova V, Habeck A, Bronstert A. 2006. Integrating wetlands and riparian zones in river basin modelling. *Ecological Modelling* **199**: 379–392.

Hayashi M, Rosenberry DO. 2002. Effects of ground water exchange on hydrology and ecology of surface water. *Ground Water* **40**: 309–316.

Hejzlar J, Anthony S, Arheimer B, Behrendt H, Bouraoui F, Grizzetti B, Groenendijk P, Jeuken MHJL, Johnsson H, Lo Porto A, Kronvang B, Panagopoulos Y, Siderius C, Silgram M, Venohr M, Zaloudik J. 2009. Nitrogen and phosphorus retention in surface waters: an inter-comparison of predictions by catchment models of different complexity. *Journal Environmental Monitoring* **11**(3): 584–593.

Hesse F, Radu FA, Thullner M, Attinger S. 2009. Upscaling of the advection-diffusion-reaction equation with Monod reaction. *Advances in Water Resources* **32**(8): 1336–1351.

Hesser FB, Franko U, Rode M. 2010. Spatially distributed lateral nitrate transport at the catchment scale. *Journal of Environmental Quality* **39**: 193–203.

Higdon D, Kennedy M, Cavendish JC, Cafeo JA, Ryne RD. 2004. Combining field data and computer simulations for calibration and prediction. *SIAM Journal on Scientific Computing* **26**: 448–466.

Huang Sh, Hesse C, Krysanova V, Hattermann F. 2009. From meso- to macro-scale dynamic water quality modelling for the assessment of land use change scenarios. *Ecological Modelling* **220**(19): 2543–2558.

Huard D, Mailhot A. 2006. A Bayesian perspective on input uncertainty in model calibration: application to hydrological model "abc". *Water Resources Research* **42**(7): W07416.

Hughes JP, Guttorp P. 1994. Incorporating spatial dependence and atmospheric data in a model of precipitation. *Journal of Applied Meteorology* **33**(12): 1503–1515.

Ibisch RB, Borchardt D, Seydell I. 2006. Influence of periphyton biomass dynamics on biological colmation processes in the hyporheic zone of a gravel bed river (River Lahn, Germany). *Advances in Limnology* **61**: 87–104.

Ingendahl D, ter Haseborg E, van der Most O, Werner D. 2009. Influence of interstitial flow velocity on hyporheic oxygen consumption and nitrate production. *Advances in Limnology* **61**: 119–137.

Isermann K. 1990. Share of agriculture in nitrogen and phosphorus emissions into the surface waters of Western Europe against the background of their eutrophication. *Fertilizer Research* **26**: 253.

Jansen MJW, Hagenaars TJ. 2004. Calibration in a Bayesian modeling framework. In *Bayesian Statistics and Quality Modeling in the Agro-Food Production Chain*, Van Boekel MAJS, Stein A, Van Bruggen AHC (eds). Kluwer: Dordrecht; 47–55.

Janssen GMCM, Cirpka OA, van der Zee SEATM. 2006. Stochastic analysis of nonlinear biodegradation in regimes controlled by both chromatographic and dispersive mixing. *Water Resources Research* **42**: W01417. DOI: 10.1029/2005WR004042.

Jones JB, Mulholland PJ. 2000. *Streams and Ground Waters*, Academic Press: San Diego; 425.

Kavetski D, Franks WS, Kuczera G. 2002. Confronting input uncertainty in environmental modeling. In *Calibration of Watershed Models*, *AGU Water Science and Applications Series*, vol. 6, Duan Q, Gupta HV, Sorooshian S, Rousseau AN, Turcotte R (eds). American Geophysical Union: Washington; 49–68.

Kavetski D, Kuczera G, Franks SW. 2006. Bayesian analysis of input uncertainty in hydrological models, 1. Theory. *Water Resources Research* **42**(3): W03407.

Kennedy CM, O'Hagan A. 2001. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B* **63**: 425–464.

Kralisch S, David O, Krause P. 2005. Using the Object Modeling System for hydrological model development and application. *Advances in Geosciences* **4**: 75–81.

Kronvang B, Grant R, Larsen SE, Svendsen LM, Kristensen P. 1995. Nonpoint-source nutrient losses to the aquatic environment in Denmark—impact of agriculture. *Marine Freshwater Research* **46**: 167.

Kronvang B, Behrendt H, Andersen HE, Arheimer B, Barr A, Borgvang SA, Bouraoui F, Granlund K, Grizetti B, Groenendijk P, Schwaiger E, Hejzlar J, Hoffman L, Johnsson H, Panagopoulos Z, Lo Porto A, Reisser H, Schoumans OF, Anthony SG, Silgram M, Venohr M, Larsen SE. 2009. Ensemble modeling of nutrient loads and nutrient load partitioning in 17 European catchments. *Journal of Environmental Monitoring* **11**(3): 572–583.

Krysanova V, Müller-Wohlfeil DI, Becker A. 1998. Development and test of a spatially distributed hydrological/water quality model for mesoscale watersheds. *Ecological Modelling* **106**: 261–289.

Kuczera G, Parent E. 1998. Monte Carlo assessment of parameter uncertainty in conceptual catchment models: the Metropolis algorithm. *Journal of Hydrology* **211**: 1–4.

Leavesley GH, Markstrom SL, Viger RJ. 2006. USGS Modular Modeling System (MMS)—Precipitation-Runoff Modeling System (PRMS) MMS-PRMS. In *Watershed Models*, Singh V, Frevert D (eds). CRC Press: Boca Raton, FL; 159–177.

Lindenschmidt KE. 2006. The effect of complexity on parameter sensitivity and model uncertainty in river water quality modeling. *Ecological Modeling* **190**(1–2): 72–86.

Lindgren GA, Destouni G. 2004. Nitrogen loss rates in streams: scale-dependence and up-scaling methodology. *Geophysical Research Letters* **31**: 13.

Marshall LA, Sharma D, Nott J. 2006. Modeling the catchment via mixtures: issues of model specification and validation. *Water Resources Research* **42**: W11409. DOI: 10.1029/2005WR004613.

McIntyre N, Lee H, Wheater HS, Young AR. 2005. Ensemle predictions of runoff in ungauged catchments. *Water Resources Research* **41**: W12434.

Meeussen JCL. 1992. *Chemical Speciation and Behaviour of Cyanide Contaminated Soil*, PhD thesis, Wageningen University.

Meeussen JCL. 2003. ORCHESTRA: an object-oriented framework for implementing chemical equilibrium models. *Environmental Science and Technology* **37**(6): 1175–1182.

Mermillod-Blondin F, Creuzè Des Chatelliers M, Gèrino M, Gaudet JP. 2000. Testing the effect of *Limnodrilus* sp. (Oligochaeta, Tubificidae) on organic matter and nutrient processing in the hyporheic zone: a microcosm method. *Archive of Hydrobiology* **149**: 467–488.

Migliaccio KW, Chaubey I, Haggard BE. 2007. Evaluation of landscape an instream modeling to predict watershed nutrient yields. *Environmental Modeling and Software* **22**: 987–999.

Montanari A. 2004. Uncertainty assessment in rainfall-runoff modelling: a review. In: *Workshop: Statistical and Mathematical Methods for Hydrological analysis, Naples, Italy*.

Mulholland PJ, Helton AM, Poole GC, Hall RH, Hamilton SK, Peterson BJ, Tank JL, Ashkenas LA, Cooper LW, Dahm CN, Dodds WK, Findlay SEG, Gregory SV, Grimm NB, Johnson SL, McDowell WH, Meyer JL, Valett HM, Webster JR, Arango CP, Beaulieu JJ, Bernot MJ, Burgin AJ, Crenshaw CL, Johnson LT, Niederlehner BR, O'Brien JM, Potter JD, Sheibley RW, Sobota DJ, Thomas SM. 2008. Stream denitrification across biomes and its response to anthropogenic nitrate loading. *Nature* **452**: 202–206.

Naegeli MW, Uehlinger U. 1997. Contribution of the hyporheic zone to ecosystem metabolism in a prealpine gravel-bed river. *Journal of the North American Benthological Society* **16**: 794–804.

Neuman S. 2003. Maximum likelihood Bayesian averaging of uncertain model predictions. *Stochastic Environmental Research and Risk Assessment* **17**: 291–305.

Omlin M, Reichert P. 1999. A comparison of techniques for the estimation of model prediction uncertainty. *Ecological Modelling* **115**: 45–59.

Omlin M, Brun R, Reichert P. 2001. Biogeochemical model of lake Zürich, sensitivity, identifiability and uncertainty analysis. *Ecological Modelling* **141**: 105–123.

Parkhurst DL, Appelo CAJ. 1999. *User's guide to PHREEQC (version 2)–A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations:*, US Geological Survey Water-Resources Investigations Report 99–4259, 312.

Petersen JE, Englund G. 2005. Dimensional approaches to designing better experimental ecosystems: a practitioner's guide with examples. *Oecologia* **145**: 216–224.

Pusch M. 1996. The metabolism of organic matter in the hyporheic zone of a mountain stream, and its spatial distribution. *Hydrobiologia* **323**: 107–118.

Rassam DW, Pagendam DE, Hunter HM. 2008. Conceptualisation and application of models for groundwater-surface water interaction and nitrate attenuation potential in riparian zones. *Environmental Modeling and Software* **23**: 859–875.

Refsgaard JC. 2007. *Hydrological Modeling and River Basin Management*, Doctoral Thesis Geological Survey of Denmark and Greenland, 90.

Refsgaard JC, van der Sluijs JP, Hojberg AL, Vanrolleghem PA. 2007. Uncertainty in the environmental modeling process—a framework and guidance. *Environmental Modeling and Software* **22**(11): 1543–1556.

Reichert P, Omlin M. 1997. On the usefulness of overparameterized ecological models. *Ecological Modelling* **95**: 289–299.

Reichert P, Borchardt D, Henze M, Rauch W, Shanahan P, Somlyódy L, Vanrolleghem P. 2001. *River Water Quality Model No. 1*, IWA—Scientific and Technical Report No.12.

Rinaldo A, Marani A. 1987. Basin scale model of solute transport. *Water Resources Research* **23**: 2107–2118.

Rinaldo A, Marani A, Bellin A. 1989. On mass response functions. *Water Resources Research* **25**(7): 1603–1617.

Rode M, Suhr U. 2007. Uncertainties in selected river water quality data. *Hydrology and Earth System Sciences* **11**(2): 863–874.

Rode M, Suhr U, Wriedt G. 2007. Multi-objective calibration of a river water quality model-information content of calibration data. *Ecological Modelling* **204**: 129–142.

Rode M, Thiel E, Franko U, Wenk G, Hesser F. 2009. Impact of selected agricultural management options on the reduction of nitrogen loads in three representative meso scale catchments in Central Germany. *Science of the Total Environment* **407**: 3459–3472.

Runkel RL. 2007. Toward a transport-based analysis of nutrient spiraling and uptake in streams. *Limnology and Oceanography—Methods* **5**: 50–62.

Runkel RL, McKnight DM, Rajaram H. 2003. Modeling of hyporheic zone processes. *Advances in Water Resources* **26**(9): 901–905.

Schälchli U. 1993. *Die Kolmation von Fließgewässersohlen: Prozesse und Berechnungsgrundlagen*—Mitteilungen der Versuchsanstalt für Wasserbau, Hydrologie und Glaziologie (VAW), Eidgenössische Technische Hochschule Zürich, 124, 273. pp.

Schmidt J, Borchardt D, Ibisch RB, Bohle HW. 2009. Direct measurement of respiration and decolmation activity of hyporheic meiofauna: first results from a new approach using anesthetizing substances. *Advances in Limnology* **61**: 185–203.

Schoumans OF, Silgram M, Walvoort DJJ, Groenendijk P, Bouraoui F, Andersen HE, Lo Porto A, Reisser H, Le Gall G, Anthony SG, Arheimer B, Johnsson H, Panagopoulos Y, Mimikou M, Zweynert U, Behrendt H, Borgvang SA. 2009. Description of nine nutrient loss models: capabilities and suitability based on their characteristics. *Journal Environmental Monitoring* **11**(3): 506–514.

Sebestyen SD, Schneider RL. 2004. Seepage patterns, pore water, and aquatic plants: hydrological and biogeochemical relationships in lakes. *Biogeochemistry* **68**: 383–409.

Seitzinger SP, Styles RV, Boyer EW, Alexander RB, Billen G, Howarth RW, Mayer B, van Breemen N. 2002. Nitrogen retention in

rivers: model development and application to watersheds in the northeastern USA. *Biogeochemistry* **57/58**: 199.

Sengschmitt D, Steiner KH, Blascke P, Gutknecht D. 1999. Selbstdichtungsvorgänge im Stauraum Wien—Freudenau.—Perspektiven—10 Jahre Gewässergüteforschung. *Neue Donau* **2–3**: 46–49.

Sheibley RW, Jackman AP, Duff JH, Triska FJ. 2003. Numerical modeling of coupled nitrification-denitrification in sediment perfusion cores from the hyporheic zone of Shingobee River, MN. *Advances in Water Resources* **26**: 977–987.

Snowling SD, Kramer JR. 2001. Evaluating modeling uncertainty for model selection. *Ecological Modeling* **138**(1): 17–30.

Szegedi K, Vetterlein D, Nietfeld H, Jahn R, and Neue H-U. 2008. The new tool rhizomath for modeling coupled transport and speciation in the rhizosphere. *Vadose Zone Journal* **7**: (Special Issue Vadose Zone Modeling): 712–720.

Thiemann M, Trosset M, Gupta H, Sorooshian S. 2001. Bayesian recursive parameter estimation for hydrologic models. *Water Resources Research* **37**: 2521–2535.

Tinker PB, Nye PH. 2000. *Solute movement in the rhizosphere,* Oxford University Press: Oxford; 444. ISBN: 0195124928.

Tomassini L, Reichert P, Knutti R, Stocker TF, Borsuk ME. 2007. Robust Bayesian uncertainty analysis of climate system properties using markov chain Monte Carlo methods. *Journal of Climate* **20**: 1239–1254.

Van der Ploeg MJ, van Wijnen T. 2009. *Interpretation of the mass response of a small Dutch catchment*, Internal Report, Wageningen University, Ecohydrology Group, 12.

Van der Velde Y, Rozemeijer JC, de Rooij GH, van Geer and FC, Broers HP. 2009a. Field-scale measurements for separation of catchment discharge into flow route contributions. *Vadose Zone Journal* DOI:10.2136/vzj2008.0141.

Van der Velde Y, de Rooij and GH, Torfs PJJF. 2009b. Catchment-scale non-linear groundwater-surface water interactions in densely drained lowland catchments. *Hydrology and Earth System Sciences* **13**: 1867–1885. www.hydrol-earth-syst-sci.net/13/1867/2009/.

Van der Zee SEATM. 1990. Analytical traveling wave solution for transport with nonlinear and nonequilibrium adsorption. *Water Resources Research* **26**(10): 2563–2578, 27(5): 983.

Van Duijn CJ, Knabner P. 1992. Traveling waves in the transport of reactive solutes through porous media, Adsorption and ion exchange part 1. *Transport in Porous Media* **8**: 167–194.

Van Griensven A, Meixner T. 2004. Dealing with unidentifiable sources of uncertainty within environmental models. In *iEMSs 2004 International Congress: Complexity and Integrated Resources Management*, Pahl C, Schmidt S, Jakeman T (eds). International Environmental Modeling and Software Society: Osnabrück, Germany; June 2004.

Van Griensven A, Meixner T, Grunwald S, Bishop T, Di Luzio M, Srinivasan R. 2006. A global sensitivity analysis method for the parameters of multi-variable watershed models. *Journal of Hydrology* **324**(1–4): 10–23.

Vandenberghe V, van Griensven A, Bauwens W. 2001. Sensitivity analysis and calibration of the parameters of ESWAT: application to the river Dender. *Water Sciences and Technology* **43**(7): 295–301.

Vandenberghe V, van Griensven A, Bauwens W. 2002. Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT. *Water Sciences and Technology* **46**(3): 1–7.

Viney NR, Croke BFW, Breuer L, Bormann H, Bronstert A, Frede H, Gräff T, Hubrechts L, Huisman JA, Jakeman AJ, Kite GW, Lanini J, Leavesley G, Lettenmaier DP, Lindström G, Seibert J, Sivapalan M, Willems P. 2005. Ensemble modeling of the hydrological impacts of land use change. In *Int. Congress on Modeling and Simulation 2005, Melbourne, Vic., Aust.*; 2967–2973.

Wagener T. 2003. Evaluation of catchment models. *Hydrological Processes* **17**: 3375–3378.

Wagener T, Gupta HV. 2005. Model identification for hydrological forecasting under uncertainty. *Stochastic Environmental Research and Risk Assessment* **19**(6): 378–387.

Wagener T, Sivapalan M, Troch P, Woods R. 2007. Catchment classification and hydrologic similarity. *Geographic Compass* **1/4**: 901–931.

Wagenschein D, Rode M. 2008. Modeling the impact of river morphology on nitrogen retention—a case study of the Weisse Elster River (Germany). *Ecological Modelling* **211**(1–2): 224–232.

Ward JV, Bretschko G, Brunke M, Danielopol D, Gibert J, Gonser T, Hildrew AG. 1998. The boundaries of river systems: the metazoan perspective. *Freshwater Biology* **40**: 531–569.

Wendland F, Albert H, Bach M, Schmidt R. 1993. *Atlas zum Nitratstrom in der Bundesrepublik Deutschland*. Springer Verlag: Berlin, Heidelberg, New York, 96 p.

Whiley M, Wilson SP. 2004. Parallel algorithms for Markov chain Monte Carlo methods in latent spatial Gaussian models. *Statistical Computation* **14**: 171–179.

Wikle CK. 2003. Hierarchical models in environmental science. *International Statistical Review* **71**(2): 181–199.

Wikle CK, Berliner LM. 2005. Combining information across spatial scales. *Technometrics* **47**(1): 80–91.

Wikle CK, Milliff RF, Nychka D, Berliner LM. 2001. Spatiotemporal hierarchical Bayesian modeling: Tropical ocean surface winds. *Journal of the American Statistical Association* **96**(454): 382–397.

Withers PJA, Jarvie HP. 2008. Delivery and cycling of phosphorus in rivers: a review. *Science of the Total Environment* **400**(1–3): 379–395.

Wollheim WM, Vörösmarty CJ, Peterson BJ, Seitzinger SP, Hopkinson CS. 2006. Relationship between river size and nutrient removal. *Geophysical Research Letters* **33**: L06410. DOI: 10.1029/2006GL025845.

Woods RA. 2003. The relative roles of climate, soil, vegetation and topography in determining seasonal and long-term catchment dynamics. *Advances in Water Resources* **26**(3): 295–309.

Wriedt G, Rode M. 2006. Modeling the Fate of nitrate in a lowland catchment system. *Journal of Hydrology* **328**(1–2): 157–176.

Yang J, Reichert P, Abbaspour KC, Yang H. 2007. Hydrological modeling of the Chaohe Basin in China: statistical model formulation and Bayesian inference. *Journal of Hydrology* **340**(3–4): 167–182.

Zhang W, Arhonditsis GB. 2008. Predicting the frequency of water quality standard violations using Bayesian calibration of eutrophication models. *Journal of Great Lakes Research* **34**: 698–720.

Zhang W, Arhonditsis GB. 2009. A Bayesian hierarchical framework for calibrating aquatic biogeochemical models. *Ecological Modeling* **220**: 2142–2161.

